

=> d que

L8

STR

RRT 27

RRT

34

PRO 5

Cb @6

O

Ak

G1~C~NH2

O O 33



G1~C~N~G2

24 25 26 -

28 29 30 31 32

1 2 3 4

G1~C~C~O~Ak

C~G3
@7 8Ak~C~G3
9 @10 11Cb~C~G3
12 @13 14Ak~O~C~O~Ak
15 16 @17 18 19O=C~O~Ak
20 @21 22 23

'VAR G1=H/AK/6

VAR G2=7/10/13

VAR G3=17/21

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 7

CONNECT IS E3 RC AT 10

CONNECT IS E3 RC AT 13

CONNECT IS E1 RC AT 15

CONNECT IS E3 RC AT 17

CONNECT IS E1 RC AT 19

CONNECT IS E1 RC AT 23

CONNECT IS E3 RC AT 30

CONNECT IS E1 RC AT 32

CONNECT IS E1 RC AT 34

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 6

GGCAT IS UNS AT 12

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M6 C AT 6

ECOUNT IS M6 C AT 12

ECOUNT IS X12 C AT 15

ECOUNT IS X12 C AT 19

ECOUNT IS X12 C AT 23

ECOUNT IS X12 C AT 32

ECOUNT IS X12 C AT 34

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE

L10 1 SEA FILE=CASREACT SSS FUL L8 (3 REACTIONS)

=> d ibib abs crd l10

L10 ANSWER 1 OF 1 CASREACT COPYRIGHT 2003 ACS

ACCESSION NUMBER: 134:178818 CASREACT

TITLE: Process for the preparation of N-(acylamino)acid esters and N-(acylamino)acetals

INVENTOR(S): Paust, Joachim; Ernst, Hansgeorg; Kaczmarek, Reinhard; Jaedicke, Hagen

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: Eur. Pat. Appl., 11 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

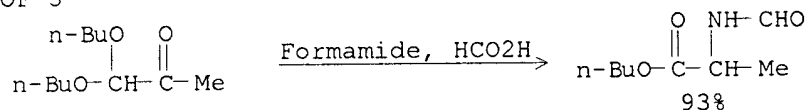
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1078916	A1	20010228	EP 2000-115618	20000720
EP 1078916	B1	20021211		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
DE 19940641	A1	20010301	DE 1999-19940641	19990826
AT 229495	E	20021215	AT 2000-115618	20000720
JP 2001072652	A2	20010321	JP 2000-252489	20000823
CN 1286246	A	20010307	CN 2000-126068	20000828
			DE 1999-19940641	19990826

PRIORITY APPLN. INFO.:

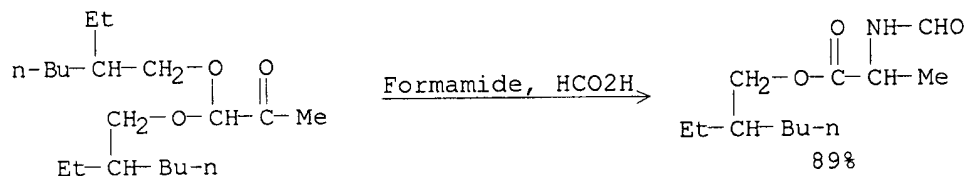
OTHER SOURCE(S): MARPAT 134:178818

AB N-acylamino acid derivs. R1CONHCH(R2)X [R1, R2 = H, C1-12 alkyl, (un)substituted aryl; X = CH(OR3)2, CO2R3; R3 = C1-12 alkyl] (e.g., N-formyl-D,L-alanine Bu ester) are prep'd. by the reaction of carboxamides R1CONH2 (e.g., formamide) with a glyoxal monoacetal deriv. R2COCH(OR3)2 (e.g., methylglyoxal dibutylacetal) in the presence of an aliph. carboxylic acid R4CO2H (R4 = C1-12 alkyl) (e.g., formic acid).

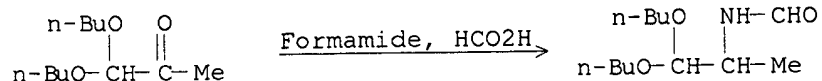
RX(1) OF 3



RX(2) OF 3



RX(3) OF 3



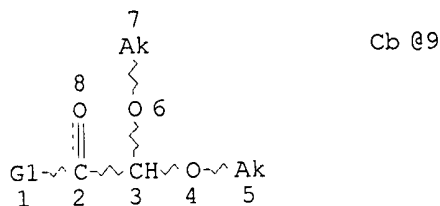
NOTE: lower concn. of formamide and formic acid

REFERENCE COUNT:

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d que

L1 SCR 273
L2 STR

*Reactant*

VAR G1=H/AK/9

NODE ATTRIBUTES:

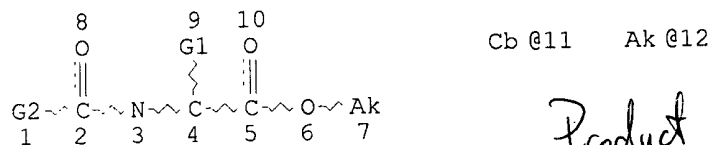
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CONNECT IS E1 RC AT 7
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 9
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS X12 C AT 5
ECOUNT IS X12 C AT 7
ECOUNT IS M6 C AT 9

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L3 SCR 278
L4 789 SEA FILE=REGISTRY SSS FUL L1 AND L3 AND L2
L5 STR

*Product*

VAR G1=AK/11

VAR G2=H/12

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 3
CONNECT IS E3 RC AT 4
CONNECT IS E1 RC AT 7
CONNECT IS E1 RC AT 12
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 11
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M6 C AT 11

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L7 485573 SEA FILE=REGISTRY ABB=ON PLU=ON NC=1 AND N/ELS AND O>1 NOT

(PMS/CI OR RSD/FA)

L9 2959 SEA FILE=REGISTRY SUB=L7 SSS FUL L5
 L11 670 SEA FILE=HCAPLUS ABB=ON PLU=ON L4(L) (RACT OR RCT OR RGT)/RL
 L12 1286 SEA FILE=HCAPLUS ABB=ON PLU=ON L9(L) PREP/RL
 L13 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 AND L12

=> d ibib abs hitstr

L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2001:152308 HCAPLUS

DOCUMENT NUMBER: 134:178818

TITLE: Process for the preparation of N-(acylamino)acid esters and N-(acylamino)acetals

INVENTOR(S): Paust, Joachim; Ernst, Hansgeorg; Kaczmarek, Reinhard; Jaedicke, Hagen

PATENT ASSIGNEE(S): BASF Aktiengesellschaft, Germany

SOURCE: Eur. Pat. Appl., 11 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1078916	A1	20010228	EP 2000-115618	20000720
EP 1078916	B1	20021211		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
DE 19940641	A1	20010301	DE 1999-19940641	19990826
AT 229495	E	20021215	AT 2000-115618	20000720
JP 2001072652	A2	20010321	JP 2000-252489	20000823
CN 1286246	A	20010307	CN 2000-126068	20000828

PRIORITY APPLN. INFO.: DE 1999-19940641 A 19990826

OTHER SOURCE(S): CASREACT 134:178818; MARPAT 134:178818

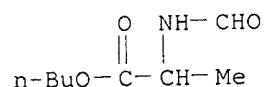
AB N-acylamino acid derivs. R1CONHCH(R2)X [R1, R2 = H, C1-12 alkyl, (un)substituted aryl; X = CH(OR3)2, CO2R3; R3 = C1-12 alkyl] (e.g., N-formyl-D,L-alanine Bu ester) are prepd. by the reaction of carboxamides R1CONH2 (e.g., formamide) with a glyoxal monoacetal deriv. R2COCH(OR3)2 (e.g., methylglyoxal dibutylacetal) in the presence of an aliph. carboxylic acid R4CO2H (R4 = C1-12 alkyl) (e.g., formic acid).

IT 86965-96-0P, N-Formyl-D,L-alanine butyl ester 326865-81-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (process for the prepn. of N-(acylamino)acid esters and N-(acylamino)acetals)

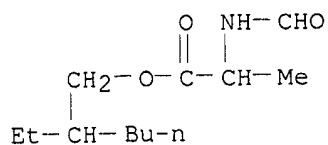
RN 86965-96-0 HCAPLUS

CN Alanine, N-formyl-, butyl ester (9CI) (CA INDEX NAME)



RN 326865-81-0 HCAPLUS

CN Alanine, N-formyl-, 2-ethylhexyl ester (9CI) (CA INDEX NAME)



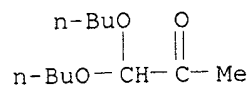
IT 19255-82-4 326865-85-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(process for the prepn. of N-(acylamino)acid esters and
N-(acylamino)acetals from)

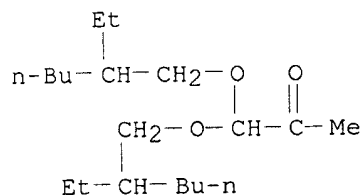
RN 19255-82-4 HCAPLUS

CN 2-Propanone, 1,1-dibutoxy- (9CI) (CA INDEX NAME)



RN 326865-85-4 HCAPLUS

CN 2-Propanone, 1,1-bis[(2-ethylhexyl)oxy]- (9CI) (CA INDEX NAME)



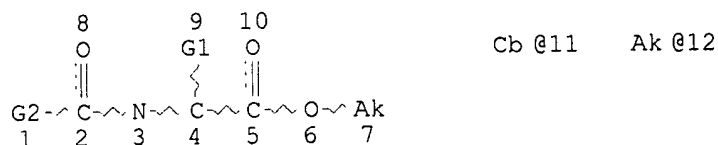
REFERENCE COUNT:

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THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d que

L2 SCR 488
L3 STR



VAR G1=AK/11

VAR G2=H/12

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 3

CONNECT IS E3 RC AT 4

CONNECT IS E1 RC AT 7

CONNECT IS E1 RC AT 12

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 11

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M6 C AT 11

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

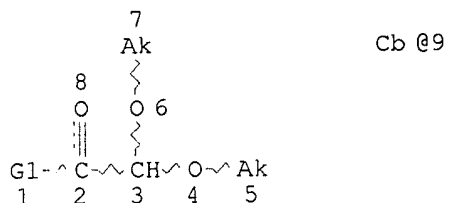
STEREO ATTRIBUTES: NONE

L6 1403829 SEA FILE=REGISTRY ABB=ON PLU=ON N/ELS AND NC=1 AND O>2 AND
NRS<2 NOT PMS/CI

L8 3266 SEA FILE=REGISTRY SUB=L6 SSS FUL L2 AND L3

L15 SCR 273

L17 STR



VAR G1=H/AK/9

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 5

CONNECT IS E1 RC AT 7

DEFAULT MLEVEL IS ATOM

GGCAT IS UNS AT 9

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS X12 C AT 5

ECOUNT IS X12 C AT 7

ECOUNT IS M6 C AT 9

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L19 SCR 278

L21 789 SEA FILE=REGISTRY SSS FUL L15 AND L19 AND L17

L22 670 SEA FILE=HCAPLUS ABB=ON PLU=ON L21(L) (RACT OR RGT OR RCT)/RL

L23 1727 SEA FILE=HCAPLUS ABB=ON PLU=ON L8(L) PREP/RL

L24 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L22 AND L23

=> d ibib abs hitstr l24 1-3

L24 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2002:391512 HCAPLUS

DOCUMENT NUMBER: 136:402027

TITLE: Preparation of amino acid derivatives for modulating
angiotensin converting enzyme-2 (ACE-2)INVENTOR(S): Acton, Susan L.; Ocain, Timothy D.; Gould, Alexandra
E.; Dales, Natalie A.; Guan, Bing; Brown, James A.;
Patane, Michael; Kadambi, Vivek J.; Solomon, Michael;
Stricker-Krongrad, Alain

PATENT ASSIGNEE(S): Millennium Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 395 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002039997	A2	20020523	WO 2001-US45703	20011031
WO 2002039997	A3	20021128		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA,
UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2002039454 A5 20020527 AU 2002-39454 20011031

PRIORITY APPLN. INFO.:

US 2000-704216 A 20001101
US 2001-870382 A 20010529
US 2001-371741P P 20011019
WO 2001-US45703 W 20011031

OTHER SOURCE(S): MARPAT 136:402027

AB ACE-2 modulating compds. Z-A-B-E (Z is a zinc coordinating moiety; E is an
enzyme coordinating moiety; A is an auxiliary pocket binding moiety; B is
a side chain binding moiety) were prepd. for the treatment of body wt.
disorders. Thus, N-[(S)- or (R)-1-carboxy-3-phenylpropyl]-L-leucine was
prepd. by the solid-phase method and showed ACE-2 inhibitory activity.

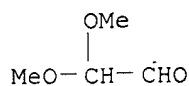
IT 51673-84-8, Glyoxal dimethyl acetal

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of amino acid derivs. for modulating angiotensin converting
enzyme-2 (ACE-2))

RN 51673-84-8 HCAPLUS

CN Acetaldehyde, dimethoxy- (9CI) (CA INDEX NAME)



IT 429664-62-0P

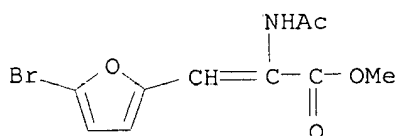
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**

(**Preparation**); RACT (Reactant or reagent)

(prepn. of amino acid derivs. for modulating angiotensin converting enzyme-2 (ACE-2))

RN 429664-62-0 HCAPLUS

CN 2-Propenoic acid, 2-(acetylamino)-3-(5-bromo-2-furanyl)-, methyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1996:545197 HCAPLUS

DOCUMENT NUMBER: 125:301538

TITLE: .alpha.-Dicarbonyls as "non-charged" arginine-directed affinity labels. Novel synthetic routes to .alpha.-dicarbonyl analogs of the PP60c-src SH2 domain-targeted phosphopeptide Ac-Tyr(OPQ3H2)-Glu-Glu-Ile-Glu

AUTHOR(S): Mehrotra, Mukund M.; Sternbach, Daniel D.; Ridriguez, Marc; Charifson, Paul; Bermán, Judd

CORPORATE SOURCE: Glaxo Wellcome Res., Research Triange Park, NC, 27709, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(16), 1941-1946

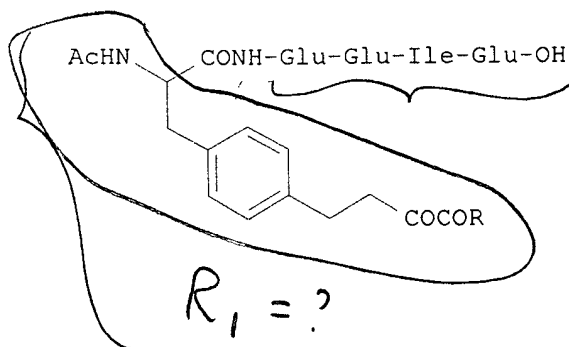
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

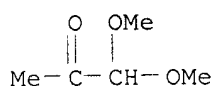


I

AB Title phosphopeptide is a potent inhibitor of pp60c-src SH2 domain mediated phosphoprotein interactions (IC50 .ltoreq. 0.5 .mu.M), but lacks cell permeability. The syntheses of its less charged analogs I (R = Me, H) are described, in which the arginine-binding phosphate group has been substituted with uncharged .alpha.-dicarbonyl moieties. The chem. described here may be of general use for the synthesis of other .alpha.-dicarbonyl compds.

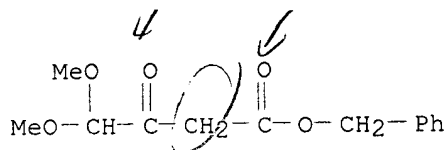
IT 6342-56-9, Pyruvic aldehyde dimethylacetal
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis of dicarbonyl analogs of PP60c-src SH2 domain-targeted phosphopeptide)

RN 6342-56-9 HCAPLUS
 CN 2-Propanone, 1,1-dimethoxy- (9CI) (CA INDEX NAME)



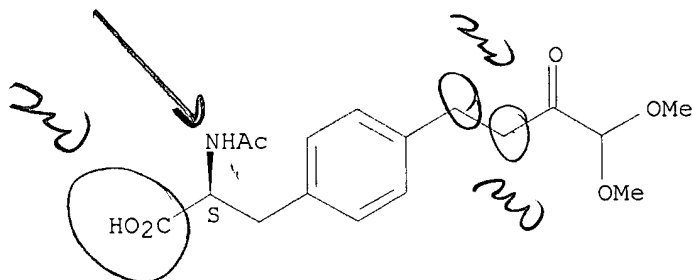
IT 182617-55-6P 182617-58-9P 182617-59-0P
 182617-60-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (synthesis of dicarbonyl analogs of PP60c-src SH2 domain-targeted phosphopeptide)

RN 182617-55-6 HCAPLUS
 CN Butanoic acid, 4,4-dimethoxy-3-oxo-, phenylmethyl ester (9CI) (CA INDEX NAME)



RN 182617-58-9 HCAPLUS
 CN L-Phenylalanine, N-acetyl-4-(4,4-dimethoxy-3-oxobutyl)- (9CI) (CA INDEX NAME)

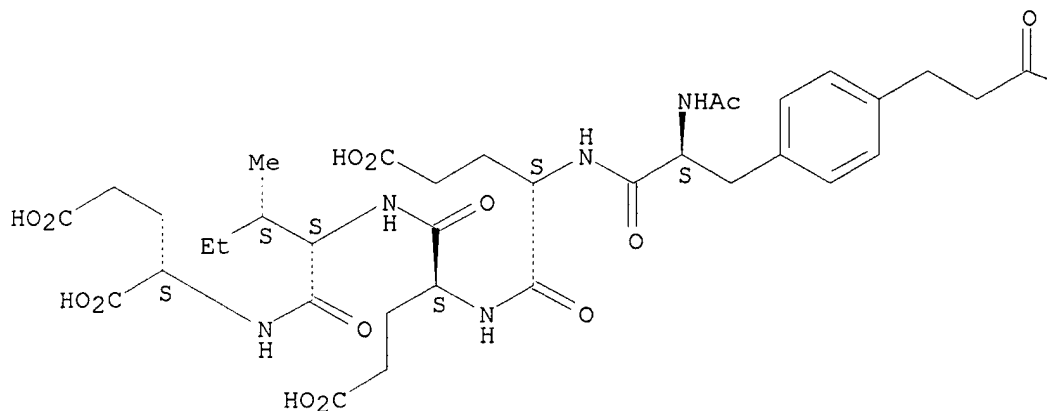
Absolute stereochemistry.



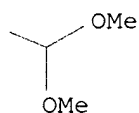
RN 182617-59-0 HCAPLUS
 CN L-Glutamic acid, N-[N-[N-[N-[N-acetyl-4-(4,4-dimethoxy-3-oxobutyl)-L-phenylalanyl]-L-.alpha.-glutamyl]-L-.alpha.-glutamyl]-L-isoleucyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



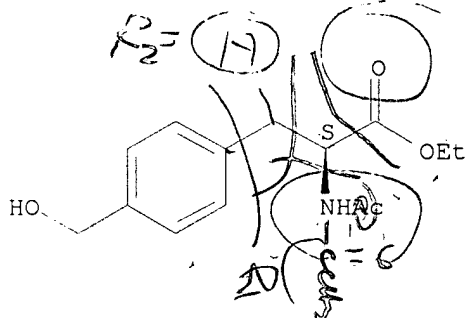
PAGE 1-B



RN 182617-60-3 HCAPLUS

CN L-Phenylalanine, N-acetyl-4-(hydroxymethyl)-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1984:51141 HCAPLUS

DOCUMENT NUMBER: 100:51141

TITLE: New syntheses and reactions in the adamantane series

AUTHOR(S): Stetter, Hermann; Mayska, Paul; Wiessner, Ulrich

CORPORATE SOURCE: Inst. Org. Chem., Rhein.-Westf. Techn. Hochsch.

Aachen, Aachen, Fed. Rep. Ger.

SOURCE: Forschungsberichte des Landes Nordrhein-Westfalen

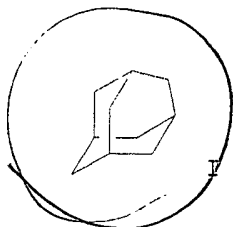
(1982), 3095, 128 pp.

CODEN: FLNWAR; ISSN: 0367-2492

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



AB An exhaustive investigation was carried out of the reactions of adamantane (I) derivs., including the use of 1-adamantyl, 1-adamantylthio, and 1-adamantylsulfinyl groups as protective groups in amino acid and peptide synthesis.

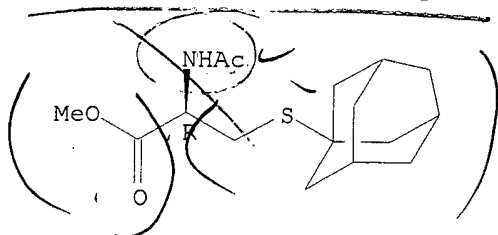
IT **88458-86-0P 88458-87-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP**
(Preparation); RACT (Reactant or reagent)
 (prepn. and deprotection and sapon. of)

RN 88458-86-0 HCAPLUS

CN L-Cysteine, N-acetyl-S-tricyclo[3.3.1.1^{3,7}]dec-1-yl-, methyl ester (9CI)
 (CA INDEX NAME)

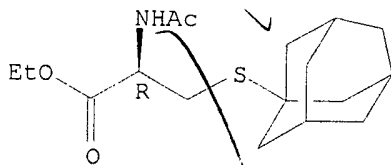
Absolute stereochemistry.



RN 88458-87-1 HCAPLUS

CN L-Cysteine, N-acetyl-S-tricyclo[3.3.1.1^{3,7}]dec-1-yl-, ethyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



IT **5344-23-0**

RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
 (reaction of, with aminoadamantane)

RN 5344-23-0 HCAPLUS

CN Acetaldehyde, diethoxy- (9CI) (CA INDEX NAME)

Reyes 09/639,681

March 3, 2003

